

Systematic errors in partially-quenched QCD plus QED lattice simulations

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At the precision reached in current lattice QCD calculations, electromagnetic effects are becoming numerically relevant. Here, electromagnetic effects are included by superimposing U(1) degrees of freedom on $N_f = 2 + 1$ QCD configurations from the Budapest-Marseille-Wuppertal Collaboration. We present preliminary results for the electromagnetic corrections to light pseudoscalars mesons masses and discuss some of the associated systematic errors.

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1. Motivation

Isospin is a near symmetry of the hadron spectrum because it is only broken by small effects:

- (i) the mass difference $m_u - m_d$
- (ii) the difference in the charge of the u and the d quark

which are summarized in the following table¹:

	u	d
Mass (MeV) [1, 2]	$2.15(03)_{\text{stat.}}(10)_{\text{sys.}}$	$4.79(07)_{\text{stat.}}(12)_{\text{sys.}}$
Charge	$\frac{2}{3}e$	$-\frac{1}{3}e$

These effects are expected to be at the percent level. The size of mass breaking is the mass difference $m_u - m_d$ relatively to a typical QCD scale Λ_{QCD} and the order of electromagnetic breaking is the fine structure constant at zero momentum $\alpha = \frac{e^2}{4\pi} \simeq \frac{1}{137}$. However, their importance is not commensurate to their size. For instance, they are responsible for the stability of matter through the proton-neutron mass difference. Moreover, lattice QCD calculations have recently approached percent or even sub-percent precision [4, 5], so the inclusion of these effects becomes relevant.

Another interesting isospin breaking quantity is the *absolute correction to Dashen's theorem*

$$\Delta_A D = \Delta_{\text{EM}} M_K^2 - \Delta_{\text{EM}} M_\pi^2 \quad (1.1)$$

where :

$$\Delta_{\text{EM}} M_P^2 = (M_{P^+}^2 - M_{P^0}^2)_{m_u=m_d} \quad (1.2)$$

is the *electromagnetic squared mass splitting* of the isospin multiplet P . One can also consider the dimensionless *relative correction to Dashen's theorem* :

$$\Delta_R D = \frac{\Delta_{\text{EM}} M_K^2}{\Delta_{\text{EM}} M_\pi^2} - 1 \quad (1.3)$$

R. Dashen has shown in [6] that $\Delta_A D = 0$ in the SU(3) chiral limit and that the leading corrections are $O(\alpha m_s, \alpha^2)$. The quantity $\Delta_A D$ is interesting because it is very sensitive to the up and down quark masses. Moreover, a precise estimation of these quantities has not been made until now (*cf.* Table 1).

2. Simulation setup

For this work, we used a subset of our 2010 SU(3) gauge configurations [2]. These configurations were generated using $N_f = 2 + 1$ QCD simulations with the tree-level Symanzik gauge action, tree level $O(a)$ -improved Wilson fermions and two steps of HEX smearing. We have already used this dataset to compute light quark masses [1, 2] and the kaon bag parameter [18].

¹We have chosen to quote the quark masses from [1, 2]. Please see [3] for a complete list of lattice determinations of these masses.

	$\Delta_A D$ (MeV ²)	$\Delta_R D$	
phenomenology	1230	0.80	Donoghue <i>et al.</i> [7] (1993)
	1300(400)	1.0(3)	Bijnens [8] (1993)
	360	0.26	Baur and Urech [9] (1996)
	1060(320)	0.9(4)	Bijnens and Prades [10] (1997)
	1080	0.68	Gao <i>et al.</i> [11] (1997)
	1070	0.74	Bijnens and Danielsson [12] (2007)
lattice	526	0.39	Duncan <i>et al.</i> [13] (1996)
	340(92)	0.30(8)	Blum <i>et al.</i> [14] (2007)
	1250(550)	N/A	Basak <i>et al.</i> [15] (2008)
	830(180)	0.60(14)	Portelli <i>et al.</i> [16] (2010)
	707(75)	0.63(6)	Blum <i>et al.</i> [17] (2010)

Table 1: Results for the violations to Dashen's theorem in phenomenology and lattice computations. Order is chronological. Bold numbers are the results given by the authors, the others are deduced from information given in the corresponding paper.

To include QED, we generate real electromagnetic fields A_μ using a non-compact formulation (*cf.* [16] for more details). Then we phase SU(3) strong links by the U(1) links $\exp(iQA_\mu)$, where Q is a chosen electric charge. The resulting U(3) links are used inside the Dirac-Wilson operator to compute quark propagators. This method allows to use previously generated SU(3) gauge configurations to obtain results, but the electromagnetic vacuum polarization is not taken into account. For the preliminary study presented here, the masses of the up and down valence quarks are tuned individually such that the bare masses are equal. This occurs when these masses become equal to the light sea quark mass [16]. The π^0 squared mass is obtained by averaging squared ground state energies obtained with $\bar{u}u$ and $\bar{d}d$ connected pseudoscalar correlators. This is correct up to NLO isospin breaking corrections.

In this setup, one is confronted with two new types of systematics effects : the quenching of the electromagnetic field and electromagnetic finite volume effects.

3. QED quenching errors

Using photon fields without vacuum polarization leads to partial quenching effects: valence quarks have electric charges but sea quarks do not. These effects can be evaluated in partially quenched chiral perturbation theory with QED (PQ χ PT+QED). Next to leading order (NLO) SU(3) formulas for self-energies and decay constants can be found in [12, 17]. The SU(3) NLO sea contribution to a pseudoscalar meson squared mass is given by :

$$\delta_{\text{sea}} M_{ij}^2 = \frac{e^2 C}{8\pi^2 F_0^4} (q_i - q_j) \sum_{s=4}^6 q_s \left[\chi_{is} \log \left(\frac{\chi_{is}}{\mu} \right) - \chi_{js} \log \left(\frac{\chi_{js}}{\mu} \right) \right] - \frac{e^2}{3} Y_1 \chi_{ij} \sum_{s=4}^6 q_s^2 \quad (3.1)$$

where i and j are the valence indices of the quarks composing the meson, indices, s , between 4 and 6 are sea quark indices, $\chi_{kl} = B_0(m_k + m_l)$, $e \simeq 0.302822$ is the positron electric charge, q_k are quark charges in units of e and Y_1 , C and F_0 are low energy constants (LECs).

For the results presented here, the sea and valence masses are very nearly equal and we can assume that the absence of sea charges is the only partial quenching effect. In that case, one can check easily that (3.1) is independent of the scale μ . The LECs C and F_0 are essentially known [12], but Y_1 , which is a sea electromagnetic contribution, is unknown. RBC, who studied other partially-quenched QED LECs [14, 17], considers that it would be unnatural that $Y_1 > 10^{-2}$. Thus, in the following, we will use $Y_1 = 10^{-2}$. With (3.1), one obtains the following partial quenching error estimates:

- negligible (less than 0.1%) for M_{K^+} , M_{K^0} , $\Delta_{\text{EM}}M_\pi$ and $\Delta_{\text{EM}}M_\pi^2$
- $\sim 0.4\%$ for M_{π^0}
- $\sim 5\%$ for $\Delta_{\text{EM}}M_K$ and $\Delta_{\text{EM}}M_K^2$

4. Electromagnetic finite volume effects

It is already known [2, p. 18] that the Budapest-Marseille-Wuppertal gauge ensembles have spatial volumes that allow to neglect QCD finite volume effects. However, as electromagnetism is a long range interaction, one might expect large QED finite volume effects on a periodic lattice. Predictions for these effects have been made in PQ χ PT+QED [19, 17]. These formulas are far from simple and complicate chiral fits. Additionally, their predictivity seems limited [17, p. 16].

Here we choose a more straightforward approach. Dimensional analysis suggests that the leading finite volume correction to the splitting of a squared hadron mass, ΔM_h^2 , takes the form :

$$\Delta M_h^2(\infty) - \Delta M_h^2(L) = e^2 \frac{A}{L^2} \quad (4.1)$$

where L is the spatial extent of the lattice and A is an unknown dimensionless constant. We found, as presented in the next section, that finite volume corrections of type (4.1) fit lattice data well but are not compatible with SU(3) PQ χ PT+QED (*cf.* Figure 1).

5. Preliminary results

For this preliminary analysis, we used the $\beta = 3.31$ subset of Budapest-Marseille-Wuppertal 2-HEX gauge configurations [2]. The main features of this dataset are:

- one lattice spacing $a \simeq 0.12$ fm
- 12 pion masses from 135 MeV to 422 MeV
- 4 spatial volumes from $(2 \text{ fm})^3$ to $(5.8 \text{ fm})^3$, with $M_{\pi^0}L > 4$

To interpolate a quantity to the physical masses, we use a Taylor expansion in $M_{\pi^0}^2$ and $M_{K^+}^2 = \frac{1}{2}(M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2)$. We choose $M_{\pi^0}^2$ because it has negligible finite volume corrections compared to those in $M_{\pi^+}^2$. The lattice spacing is computed in physical units using the Ω^- baryon mass. The infinite volume extrapolation is performed by including corrections of the kind (4.1) into the fit. Fits are carried out using fully correlated χ^2 minimization and a bootstrap error analysis.

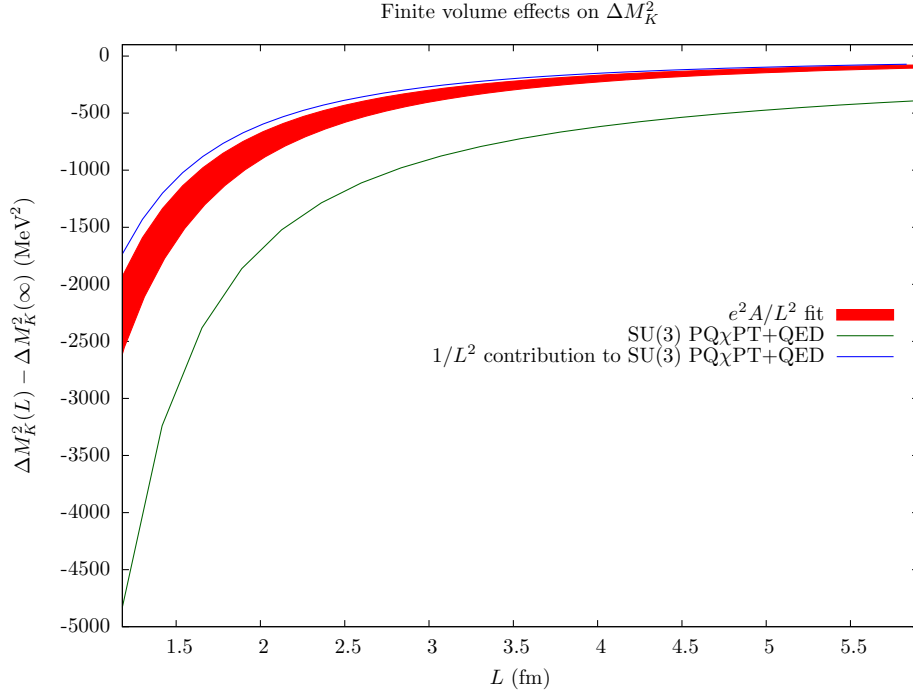


Figure 1: Comparison of our results with different models of finite volume corrections for the kaon squared mass splitting, as a function of lattice spatial extent. The red band represents the fit of our lattice data to the model (4.1), with M_{π^0} fixed to its physical value. Only statistical errors are shown. The green curve represents the prediction of SU(3) PQχPT+QED, which depends only on the LO, LECs F_0 and C , given in [12]. There is a clear disagreement between the two. However, the $\frac{1}{L^2}$ contribution from the full SU(3) PQχPT+QED expression (blue curve) roughly agrees with our data.

Using this methodology, we obtain the following preliminary results (an example of such a fit is shown in Figure 2) :

$$\Delta_{\text{EM}} M_K^2 = 2179(34)_{\text{stat.}}(100)_{\text{qu.}}(?)_{\text{sys.}} \text{ MeV}^2 \quad (5.1)$$

$$\Delta_{\text{EM}} M_\pi^2 = 1283(30)_{\text{stat.}}(0)_{\text{qu.}}(?)_{\text{sys.}} \text{ MeV}^2 \quad (5.2)$$

$$\Delta_{AD} = 896(37)_{\text{stat.}}(100)_{\text{qu.}}(?)_{\text{sys.}} \text{ MeV}^2 \quad (5.3)$$

$$\Delta_{RD} = 0.70(4)_{\text{stat.}}(8)_{\text{qu.}}(?)_{\text{sys.}} \quad (5.4)$$

where $(?)_{\text{sys.}}$ stands for the systematic errors which we have not yet estimated, such as those associated with taking the continuum limit, etc.

6. Conclusion

Using the methodology that we presented last year [16], we extended our dataset down to the physical value of the light quark mass. We also studied two important systematics effects: QED quenching and finite volume effects.

Our results are promising and close to phenomenological estimates [3]. Moreover, concerning the finite volume effects, the results are compatible with a simple $\frac{1}{L^2}$ model and it seems that SU(3) PQχPT+QED fails to describe them.

In the short term, we will continue our analysis on several lattice spacings with non-degenerate up and down quark masses. This will provide the last ingredients to define precisely the physical point, which require a continuum limit and physical isospin breaking.

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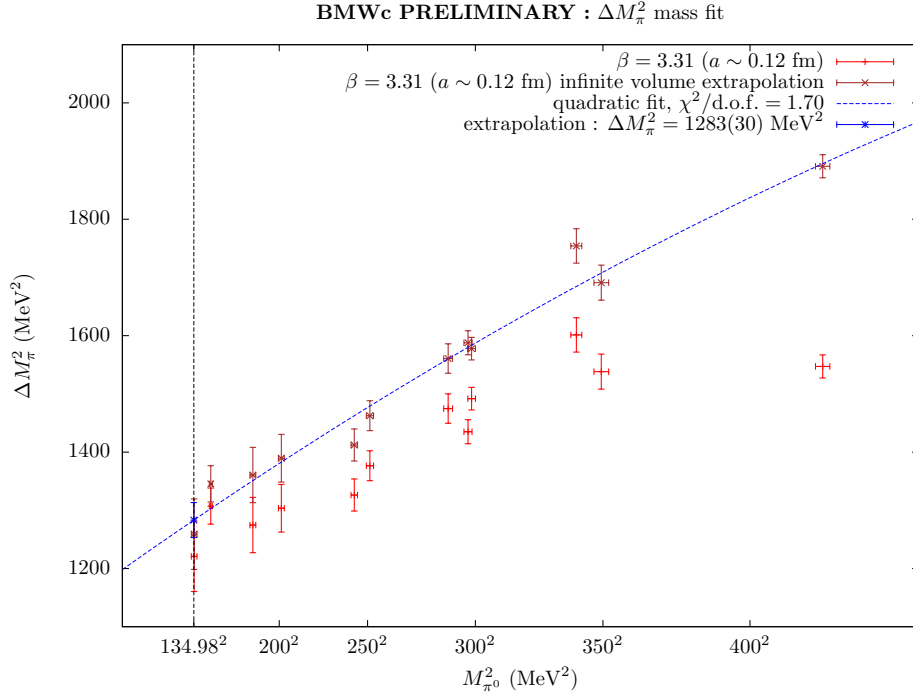


Figure 2: Pion squared mass splitting vs. neutral pion squared mass. Red points represent raw lattice data, dark red points are the same data with finite volume correction of type (4.1) and the dashed blue line is the result of the physical point fit.

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